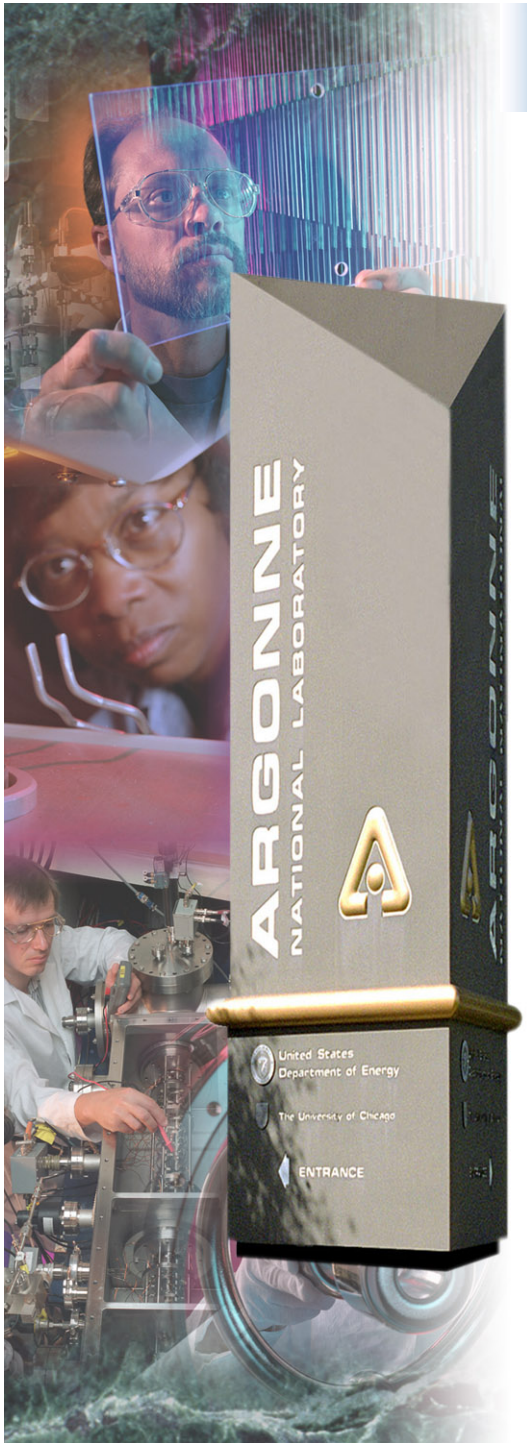

ARGONNE NATIONAL LABORATORY

Neutronic Code Development at ANL

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Motivation

- Component of a larger integrated simulation program at ANL.
  - Neutronics
  - Fuel modeling
  - Thermal hydraulics
  - Balance of plant

- The neutronic analysis of complex systems:
  - Gen IV reactors,
  - AFCI transmutation systems,
  - Space nuclear applications.

- Refined analysis for present day reactors.

Deterministic rather than Stochastic Approach

- Very accurate evaluations of detailed reaction rate distributions
- Determination of small reactivity effects
- Sensitivity and uncertainty analysis
- Systematic extrapolation to reference solutions
- Application to reactor transient and burnup problems

One Step Deterministic Approach

- Seamless approach to replace present three steps:
  - 1. Single pin cells – fine energy group structure
  - 2. Fuel assemblies – intermediate energy group structure
  - 3. Whole core – coarse energy groups
- Very large number of energy groups: ultimately ~10,000
- General geometry capability to offer the same flexibility as Monte Carlo

The proposed code: UNIC (Ultimate Neutronic Investigation Code),

- Multigroup energy discretization
- Three-dimensional finite elements in space
- Spherical harmonics, discrete ordinate and/or integral angular discretization
- Domain decomposition through incoming and outgoing angular flux distributions, allowing second- and first-order Boltzmann equation form coupling when needed.
- Initial implementation: spherical harmonics with second-order form.

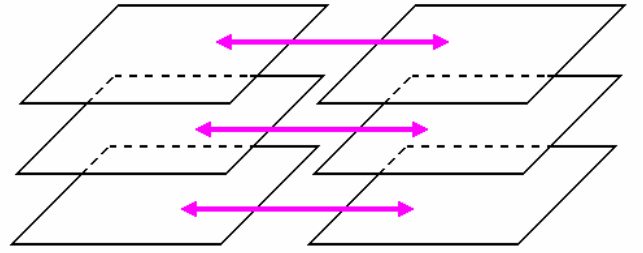
UNIC

- Problem domain divided into spatial “nodes” or subdomains. Each subdomain corresponding to a processor on a parallel computer.
- Subdomain calculations performed one per processor by sparse matrix iterative means, e.g. preconditioned conjugate gradient methods (PETSc)
- Domain decomposition method couples iterative subdomain solutions to obtain a global solution iteratively, e.g. with red-black or multicolored iteration.

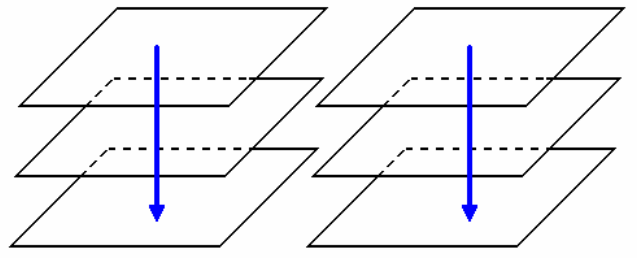
UNIC

- Three dimensional nodes of arbitrary shape must be formulated and coded, possibly with curved surfaces.

- Possible modification of iteration strategy to reduce processor to processor coupling



subdomain 1 subdomain 2
Iteration by group



subdomain 1 subdomain 2
Iteration by subdomain

UNIC – Current Status

- Reformulated the second-order form of the transport equation with incoming angular flux boundary conditions.
- Implemented second order P_n equations with isotropic scattering in Fortran 90 code with object orientated coding structure.
- The finite element mesh geometry, element solver, and element library incorporated into separate Fortran modules with minimal linkages.
- Spherical harmonics module written to handle arbitrary vacuum and reflected boundary conditions for unstructured finite element mesh geometries.
- Solver routine written for steady state multigroup eigenvalue and/or fixed source iterations for one, two, and three dimensional unstructured finite element mesh geometries.

UNIC – Current Status

- Inner iteration (linear system of equations) solver implemented based on conjugate gradient method with partial Cholesky decomposition as preconditioner for the spatial components

- Satisfactory results obtained on serial machines for standard simple benchmarks for two and three dimensional Cartesian multigroup problems

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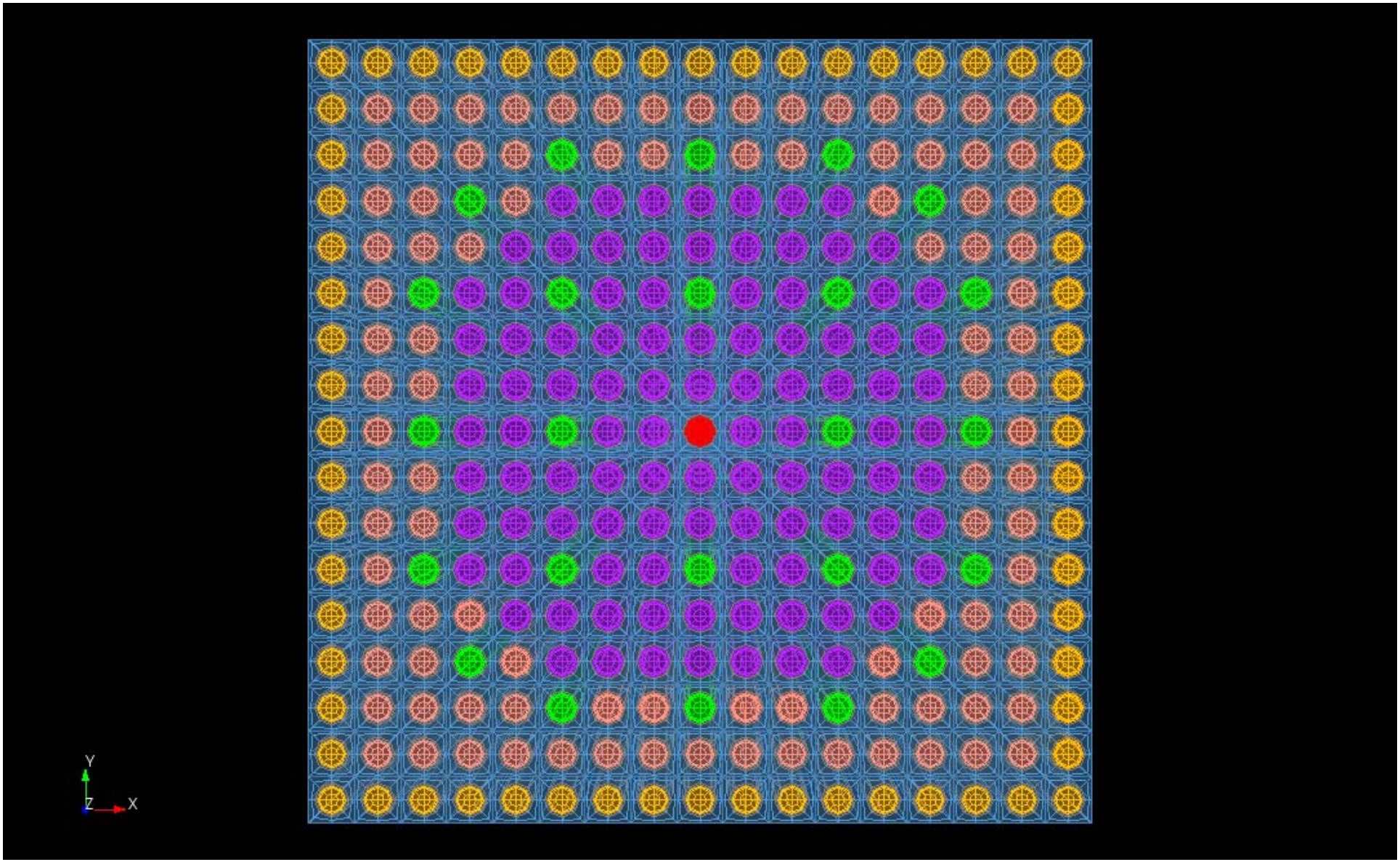
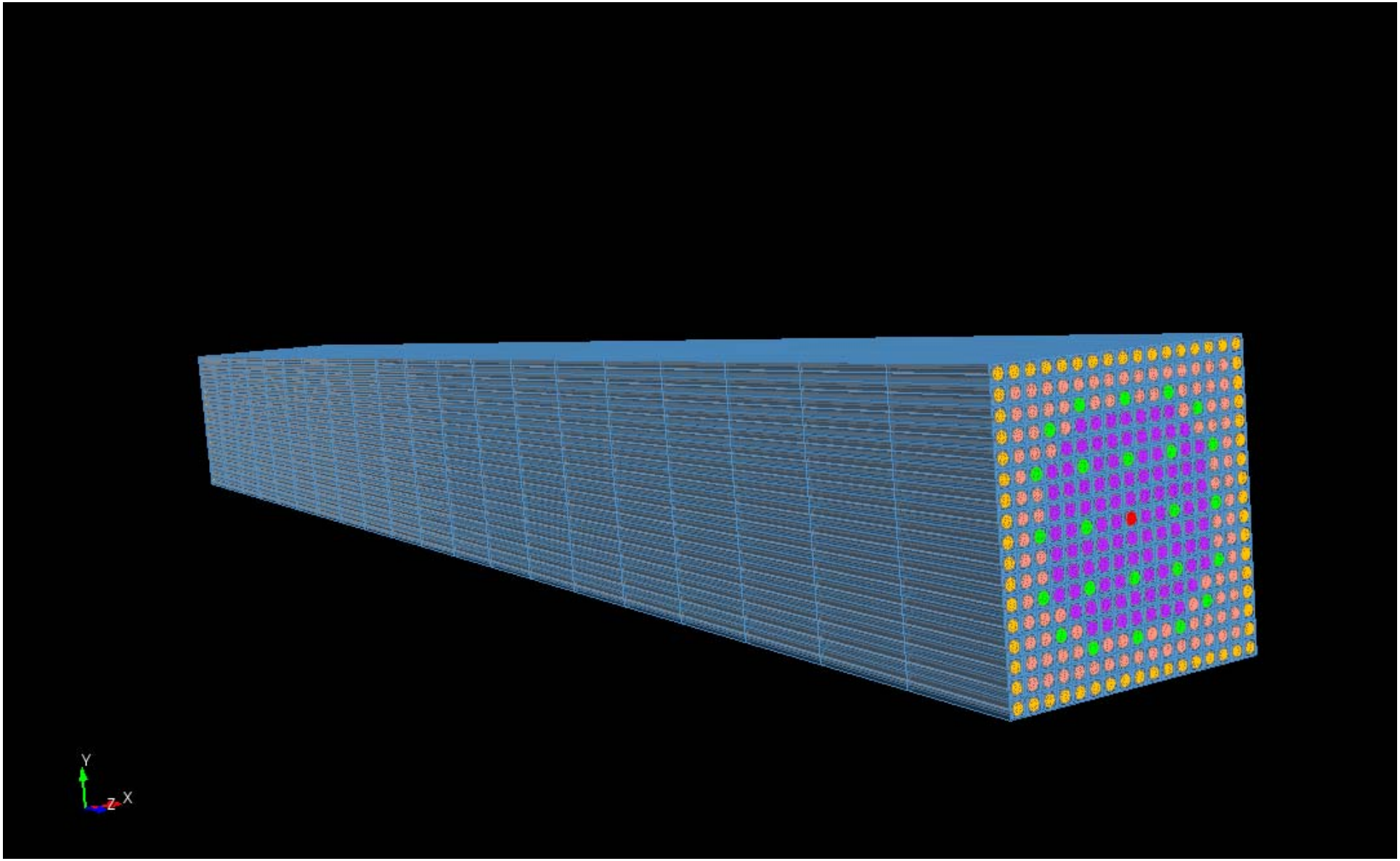
- Work begun for complex geometry mesh generation using CUBIT.

- UNIC will be integrated in SALOME to address pre- and post-processing as well of the coupling with other multi-physics modules


Y
Z
X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For the second order finite element P_n equations we start from:

$$\mathbf{A}\xi = \mathbf{q} \qquad (1)$$

with

$$\mathbf{A} = \int dV \sigma^{-1} (\nabla_k \mathbf{f}) \nabla_{k'} \mathbf{f}^T \otimes \cdot \int d\Omega \Omega_k \, \Omega_{k'} \mathbf{y}_+ \mathbf{y}_+^T + \int dV \sigma \mathbf{f}\mathbf{f}^T \otimes \mathbf{I}_\Omega - \int dV \sigma_s \mathbf{f}\mathbf{f}^T \otimes \mathbf{I}_\delta$$
$$+ \sum_\gamma \int_\gamma d\Gamma \; \mathbf{f}\,\mathbf{f}^T \otimes \int d\Omega \; \left| \hat{\Omega} \cdot \hat{n} \right| \mathbf{y}_+ \mathbf{y}_+^T$$

$$\mathbf{q} = \mathbf{s} + 2 \int d\Gamma \mathbf{f} \otimes \int_{\hat{n} \cdot \hat{\Omega} < 0} d\Omega \; |\hat{\Omega} \cdot \hat{n}| \mathbf{y}_+ \psi_\lambda \qquad (2)$$

Using partial currents:

$$\mathbf{q} = \mathbf{s} + 2\sum_{\gamma} \int_{\gamma} d\Gamma \; \mathbf{f}\,\mathbf{h}_{\gamma}^{T} \otimes \mathbf{I}_{\Omega}\,\mathbf{j}_{\gamma}^{-} \quad (3)$$

and

$$\mathbf{j}_{\gamma}^{+} = \left[\int_{\gamma} d\Gamma \; \mathbf{h}_{\gamma}\,\mathbf{h}_{\gamma}^{T}\right]^{-1} \otimes \mathbf{I}_{\Omega} \quad (4)$$

$$\cdot\left[\tfrac{1}{2}\int_{\gamma} d\Gamma \; \mathbf{h}_{\gamma}\mathbf{f}^{T} \otimes \int d\Omega \; \left|\hat{\Omega}\cdot\hat{n}_{\gamma}\right| \mathbf{y}_{+}\mathbf{y}_{+}^{T} - \tfrac{1}{2}\int_{\gamma} d\Gamma\sigma^{-1} \; \mathbf{h}_{\gamma}(\nabla_{k}\mathbf{f})^{T} \otimes \cdot\int d\Omega\Omega_{k} \; \hat{\Omega}\cdot\hat{n}_{\gamma}\,\mathbf{y}_{+}\mathbf{y}_{+}^{T}\right]\xi$$

The subdomain solution algorithm would consist of assuming the incoming flux distribution, $\mathbf{j}_{\gamma}^{-}$, is known, and calculating q from Eq. (3). Knowing, q, use Eq. (1) to calculate ξ iteratively. With ξ known, use Eq. (4) to calculate the outgoing flux distribution $\mathbf{j}_{\gamma}^{+}$.

For the discontinuous finite element S_n equation we have:

$$\mathbf{q} = \mathbf{s} + 2\sum_{\gamma} \int_{\gamma} d\Gamma \mathbf{f}\mathbf{p}_{\gamma}^{T} \sum_{\hat{n}\cdot\hat{\Omega}_i<0} w_i \,|\hat{\Omega}_i \cdot \hat{n}\,|\, \boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}_i) \otimes \mathbf{y}_{+}(\hat{\Omega}_i) \qquad (5)$$

and for the outgoing flux distribution

$$\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}_i) = \left[\int_{\gamma} d\Gamma \mathbf{p}_{\gamma}\mathbf{p}_{\gamma}^{T}\right]^{-1} \left[\int_{\gamma} d\Gamma \mathbf{p}_{\gamma}\mathbf{f}^{T} - \int_{\gamma} d\Gamma \,\tfrac{1}{\sigma}\mathbf{p}_{\gamma}\overset{\mathrm{V}}{\nabla}\mathbf{f}^{T}\cdot\hat{\Omega}_i\right] \otimes \mathbf{y}_{+}(\hat{\Omega}_i)\boldsymbol{\xi} \qquad (6)$$

To summarize the derivation, Eq. (1) is used to solve the finite-element spherical harmonic approximation within the subdomain. If the subdomain is coupled to others in which the spherical harmonic approximation is also used, then Eqs. (3) and (4) are used for the incoming and outgoing flux distributions respectively. If the adjoining subdomains are treated with discrete ordinate methods, Eqs. (5) and (6) are used for incoming and outgoing flux.